



U.S. DEPARTMENT OF
ENERGY

OFFICE OF
SCIENCE

Advanced Scientific Computing Research Program

The View from Germantown

**ALCF Getting Started Workshop
January 27-29, 2010**

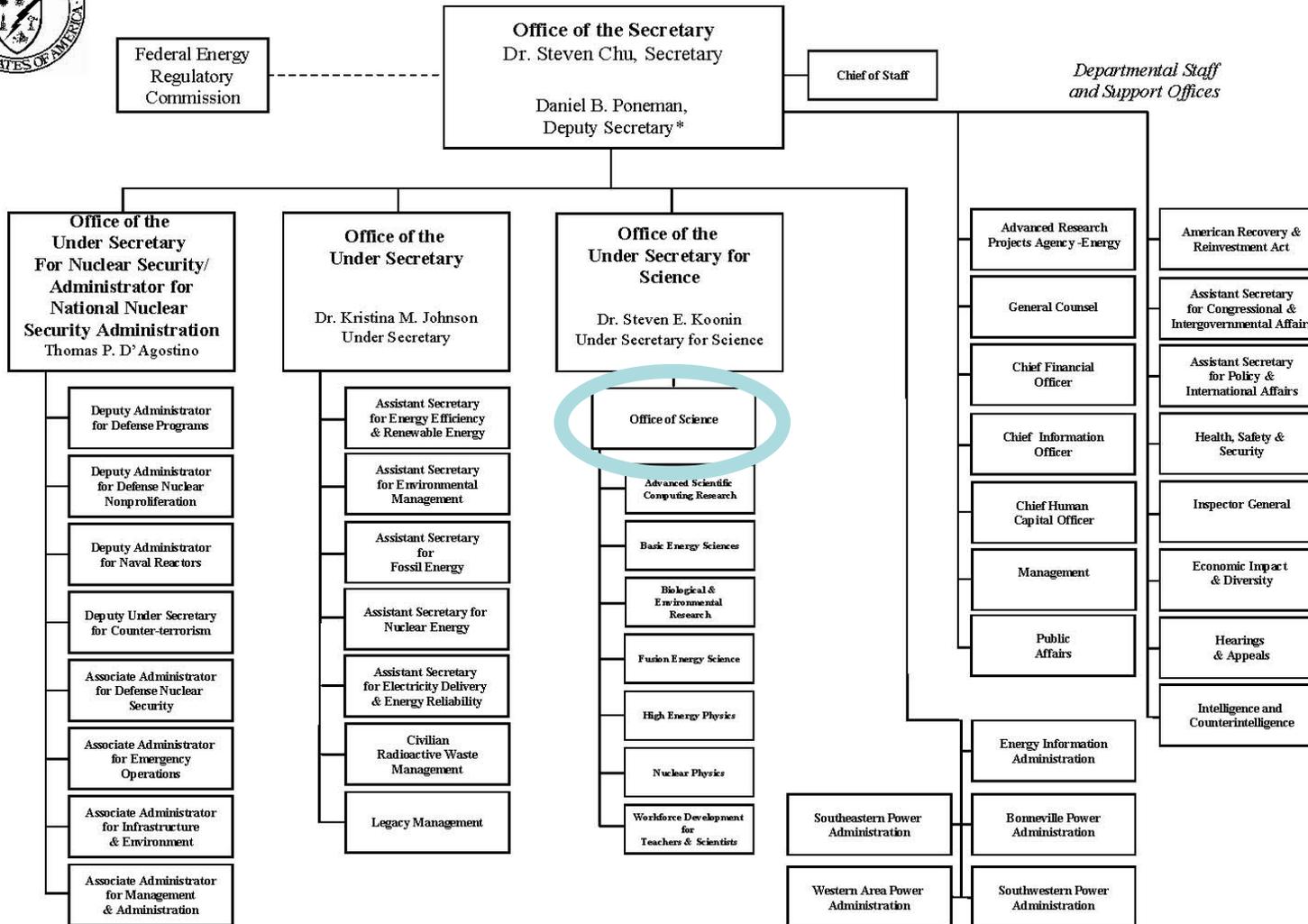
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DEPARTMENT OF ENERGY



* The Deputy Secretary also serves as the Chief Operating Officer



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ENERGY

LEADING BASIC RESEARCH
FOR A SUSTAINABLE FUTURE

ENVIRONMENT

UNDERSTANDING CLIMATE CHANGE AND
IMPROVING THE ENVIRONMENT

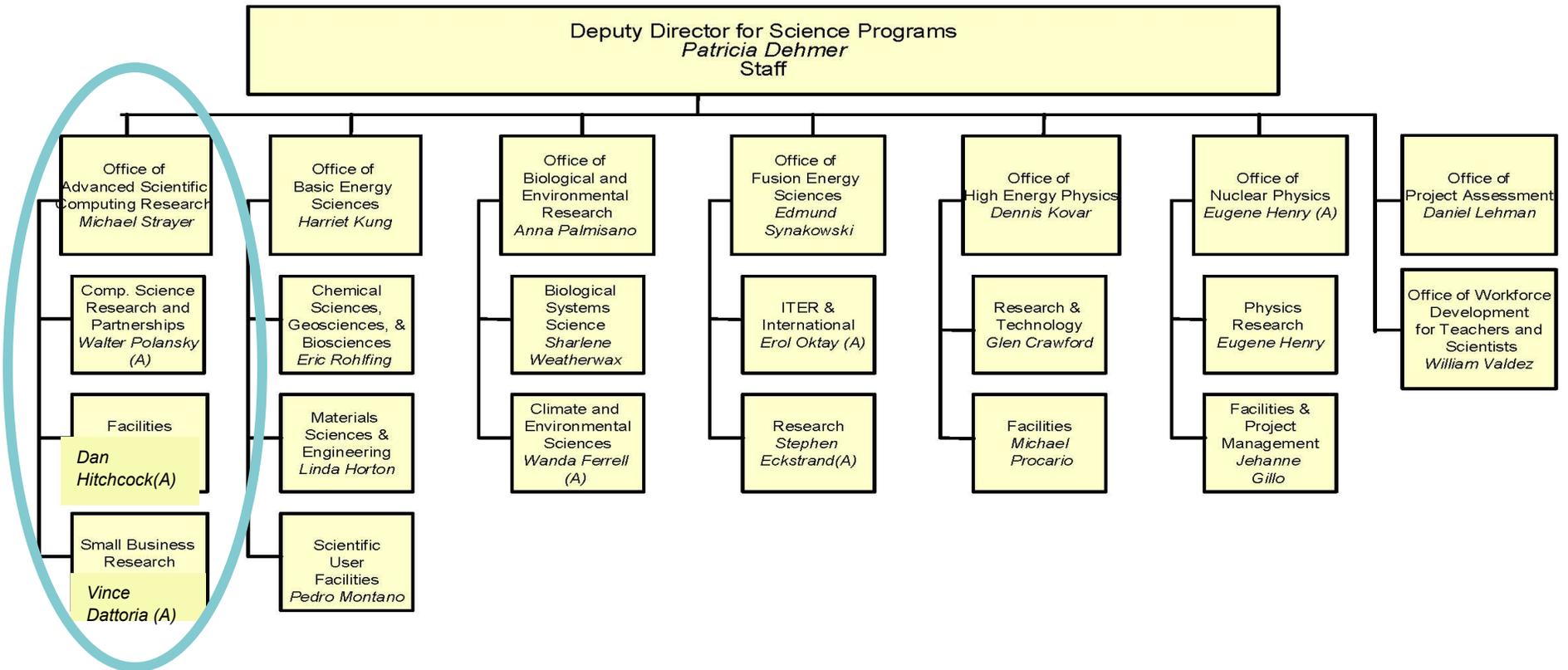
INNOVATION

BUILDING RESEARCH INFRASTRUCTURE AND
PARTNERSHIPS THAT FOSTER INNOVATION

DISCOVERY

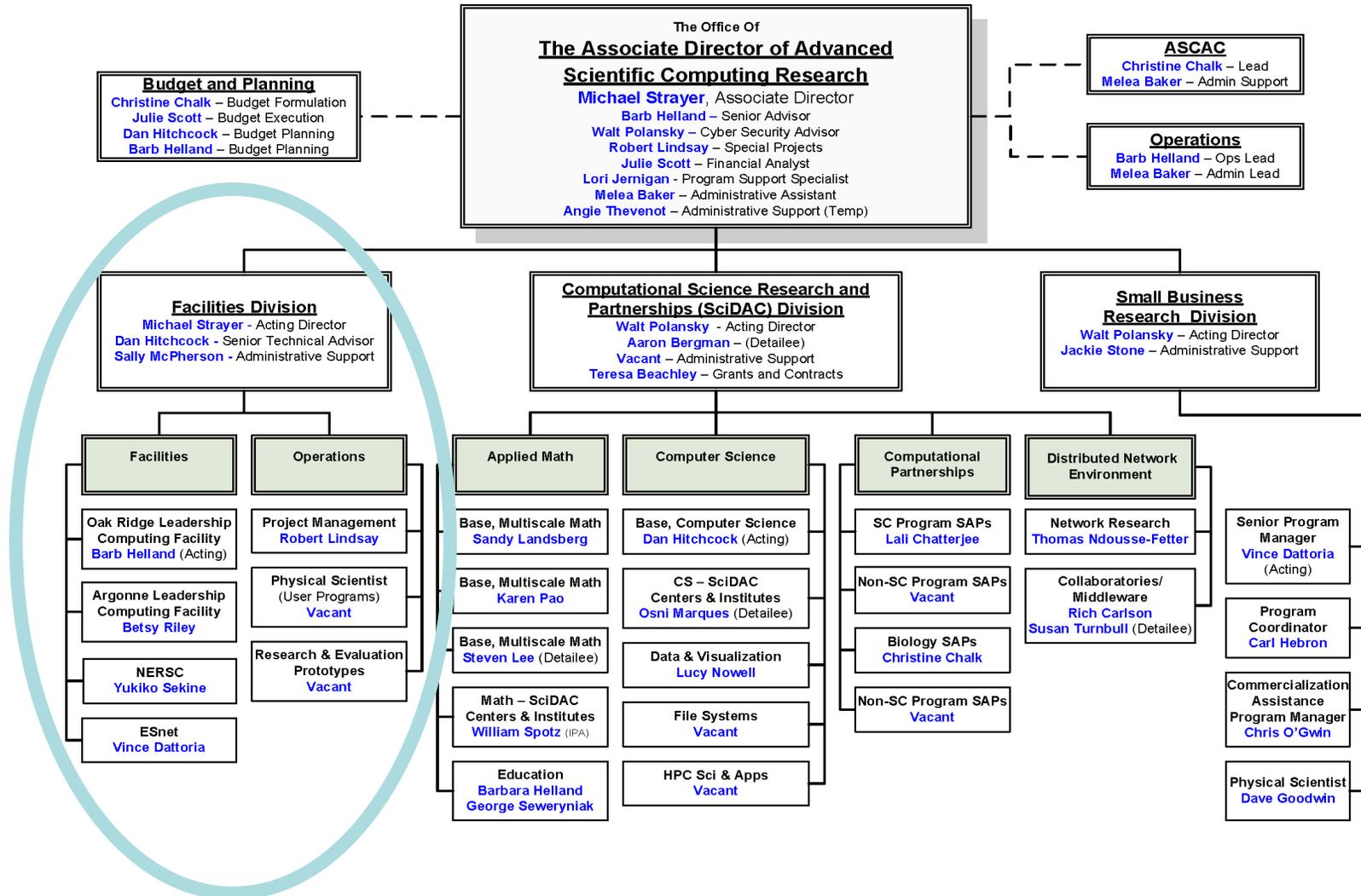
UNRAVELING NATURE'S
DEEPEST MYSTERIES

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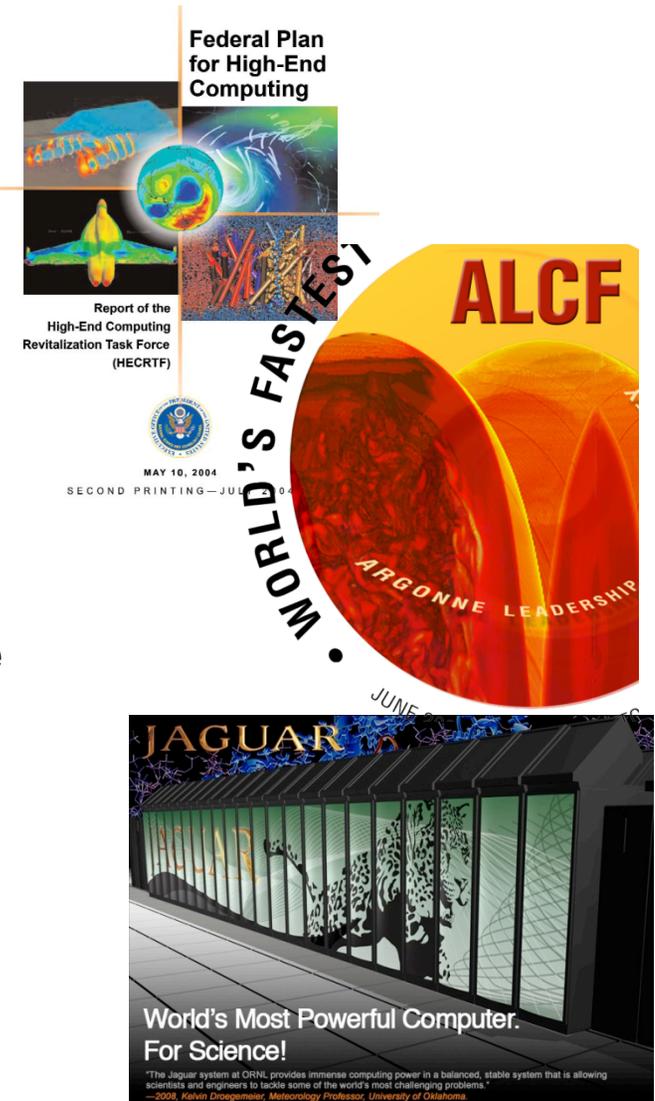
ASCR Facilities Division





ASCR Facilities Strategy

- **Providing the Tools – High-End Computing**
 - **High-Performance Production Computing** – National Energy Research Scientific Computing Center (**NERSC**) at Lawrence Berkeley National Laboratory (LBNL)
 - Delivers high-end capacity computing to entire DOE SC research community
 - **Leadership-Class Computing** – **Leadership Computing Facilities (LCFs)**
 - Argonne National Laboratory (ANL -- **ALCF**)
 - Oak Ridge National Laboratory (ORNL -- **OLCF**)
 - Deliver highest computational capability to national and international researchers through peer-reviewed **Innovative and Novel Computational Impact on Theory and Computation (INCITE)** program (80% of resources)
- **Investing in the Future - Research and Evaluation Prototypes**
- **Linking it all together – Energy Sciences Network (ESnet)**





Next Generation of LCFs

Mission need approved January 2009

“The upgrade of the Leadership Computing Facilities to tens of petaflops by the 2011-2013 timeframe is vital to the U.S. playing a leading role in several important international programs, including:

- *climate science (International Panel on Climate Change),*
- *fusion energy research (ITER), and*
- *the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program”*

- ORNL’s Cray XT5 upgraded to 2.3 PF, increasing allocatable hours by 50%
- New NERSC-6 Cray System “Hopper” will be >1PF in 3Q10
- ALCF-2 upgrade “Mira” Blue Gene/Q will be 10PF in FY12



ALCF-2 Upgrade System "Mira"



- Enables key science impact:
 - Predict abrupt regional climate change
 - Design safer, cost-effective nuclear power reactors
 - Enhancement of the extraction of biofuels from biomass
 - In silico design of nano-structured storage systems
- Builds on ASCR/NNSA investment and LLNL BG/Q Sequoia competitive bid procurement

Science Enablement Program

- 15 Science Teams
- Call: 1Q10, 1st Selection: 3Q10
- Port, Optimize, New Modeling Approaches
- Early Access to Pre-Production hardware

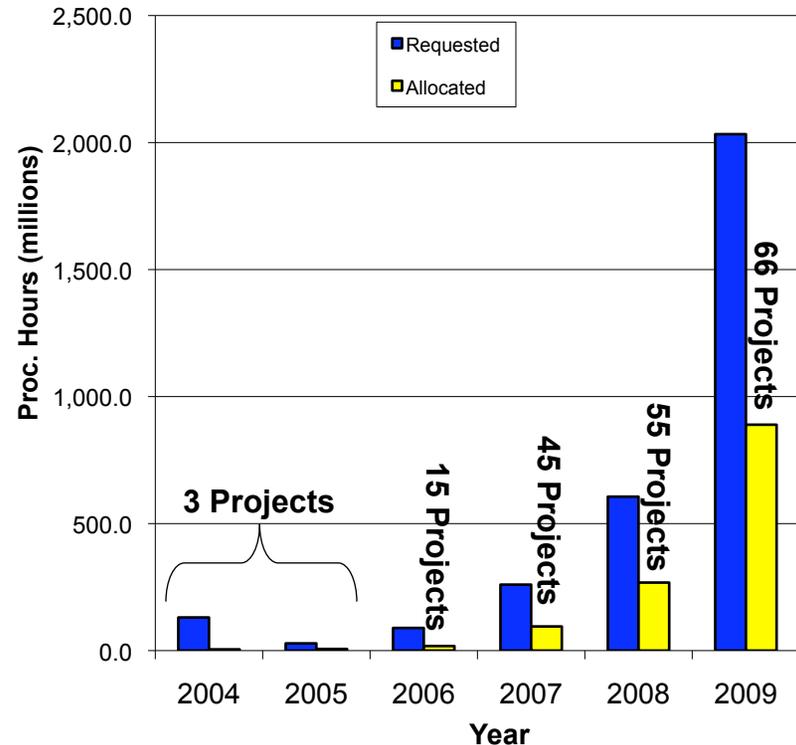
Mira Blue Gene/Q System

- 10 Pflop/s peak
- ~800K cores, 16 per chip
- ~70PB disk, ~470 GB/s I/O bandwidth
- Power efficient, water cooled

4Q10	1Q11	2Q11	3Q11	4Q11	1Q12	2Q12	3Q12	4Q12
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- Initiated in 2004 at NERSC
- Now provides Office of Science Leadership Class Computing resources to a small number of computationally intensive research projects of large scale, that can make high-impact scientific advances through the use of a large allocation of computer time and data storage
- Open to national and international researchers, including industry
- No requirement of DOE Office of Science funding
- Peer and computational readiness reviewed





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ALCF: IBM Blue Gene/P—557 TFs



Intrepid: 40,960 quad-core compute nodes (163,840 proc.), 80TB of memory

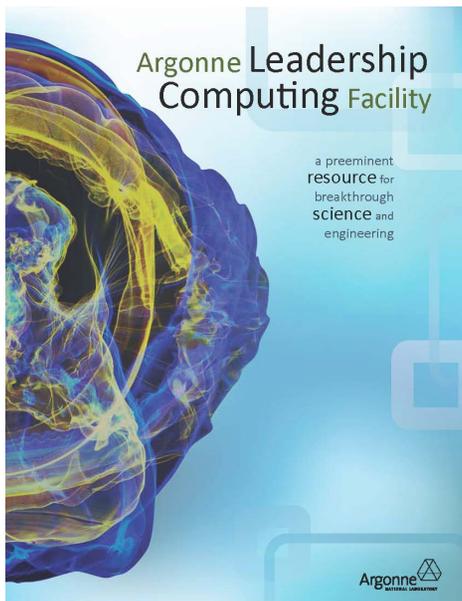


From ALCF:

- Sign ALCF User Agreements
- Adhere to ALCF Cyber Security and other computing policies
- Work with the Catalyst, Performance Engineering, and Viz & Data Analysis groups to take advantage of the IBM Blue Gene architecture
- Don't wait to start computing

From DOE:

- Share your scientific accomplishments!



Argonne Leadership Computing Facility

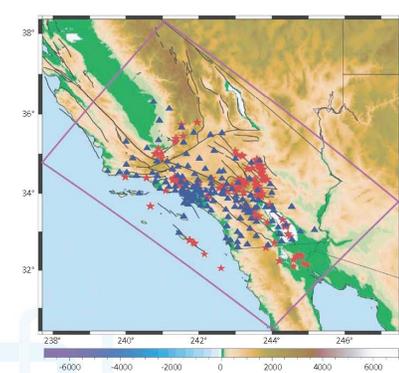
a preeminent resource for breakthrough science and engineering



INCITE Hours Allocated on the ALCF's Blue Gene/P: 5 Million

Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 2 Hz

Earthquake simulations help scientists understand the hazards posed by large future earthquakes. Before predictive simulation results for future earthquakes are scientifically acceptable, the earthquake computational models must be validated by simulating well-recorded historical earthquakes and comparing simulation results to observational data.

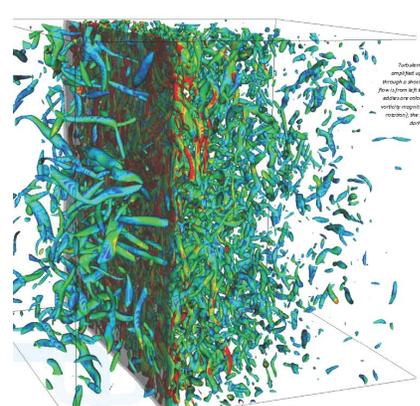


The figure shows the results of the 3-D structural model runs at the 0.2 Hz resolution. Source: (in red), with stations in blue. (Image Credit: Eric Selva, University of Wyoming)

INCITE Hours Allocated on the ALCF's Blue Gene/P: 8 Million

Fundamental Study of Shock/Turbulence Interaction

Interactions between shock waves and turbulence severely affect the stability of the flow through supersonic propulsion systems. Inadequate models—due to a poor understanding of the shock/turbulence interaction phenomena—result in designs that sacrifice performance for stable operation. A better understanding of the fundamental physics would lead to more accurate turbulence models for improved efficiency in supersonic aircraft design.

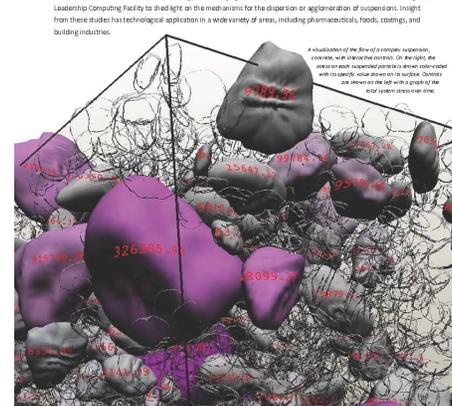


Turbulent eddies are stretched and compressed through a shock wave. The shock wave is shown in blue. The eddies are colored by their entropy (representing local temperature), the shock is the dark blue sheet.

INCITE Hours Allocated on the ALCF's Blue Gene/P: 750,000

What Insights Are Revealed When Modeling Concrete's Rheological Properties?

Study of the flow behavior of dense suspensions remains an outstanding research problem because of the immense complexity of these systems that are not tractable by simple analytic theories. Computational models are needed that account for dense packing of particles with a broad shape and size variation along with interparticle interactions. Researchers from the National Institute of Standards and Technology are leveraging the computational resources of the Blue Gene/P at the Argonne Leadership Computing Facility to shed light on the mechanisms for the dispersion or agglomeration of suspensions. Insights from these studies has technological application in a wide variety of areas, including pharmaceuticals, foods, coatings, and building industries.

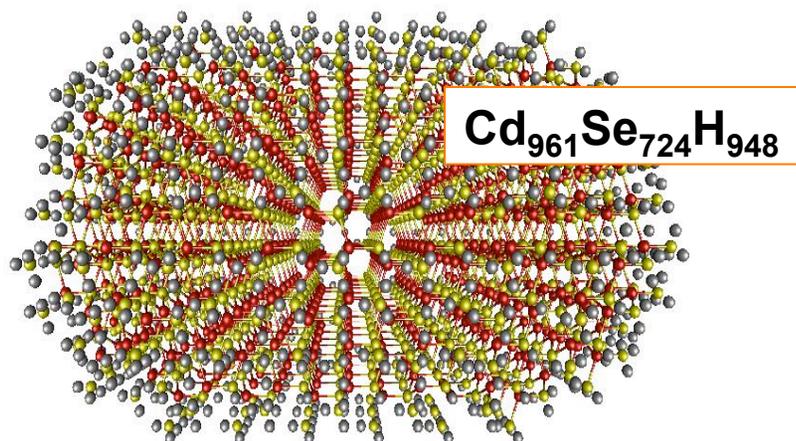


A visualization of the flow of a complex suspension, concrete, with particles in red. On the left, the particles in each sequential picture are shown color-coded with the same color scheme to indicate density. Changes are shown on the left with a gradient of the color from black to red.



Science

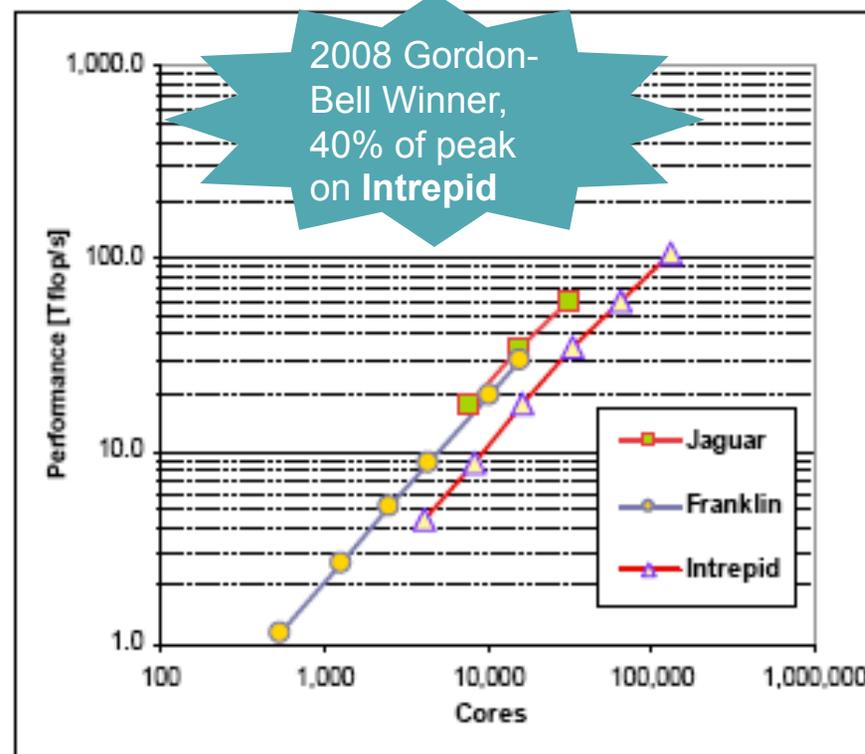
- Design better materials for products including solar cells
- *Ab initio* electronic structure calculations
- Lin-Wang Wang, B. Lee, H. Shan, Z. Zhao, J. Meza, E. Strohmaier, D. Bailey, "Linear Scaling Divide-and-conquer Electronic Structure Calculations for Thousand Atom Nanostructures," SC08, to appear.



Dipole moment calculated
on 2633 atom quantum rod

Methods and Challenges

- Novel divide & conquer approach to solve DFT but reducing $O(n^3)$ to $O(n)$
 - Many months to 30 hours
 - Direct DFT impractical
- Mapping critical
 - Linear scaling to 160K cores and a 10% improvement in





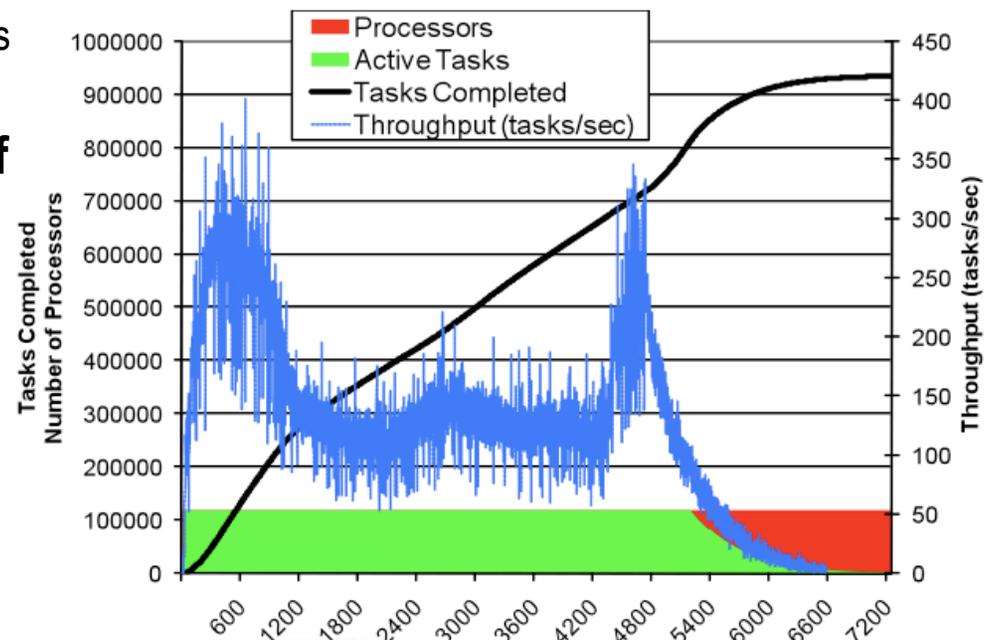
Science

- **Reduce dead ends in antibiotics and anticancer drugs with DOCK5 and DOCK6**
 - 9 enzymatic proteins in core metabolism of bacteria and humans screened against 15,351 natural compounds and existing drugs
 - Study correlations and re-prioritize proteins for further study
- **Able to complete 21.43 CPU-years of analysis in 2.01 wall-hours**

•MCS Computer Science teams, using discretionary allocation, to facilitate science
•Participated in submitting 2 INCITE proposals

Methods and Challenges

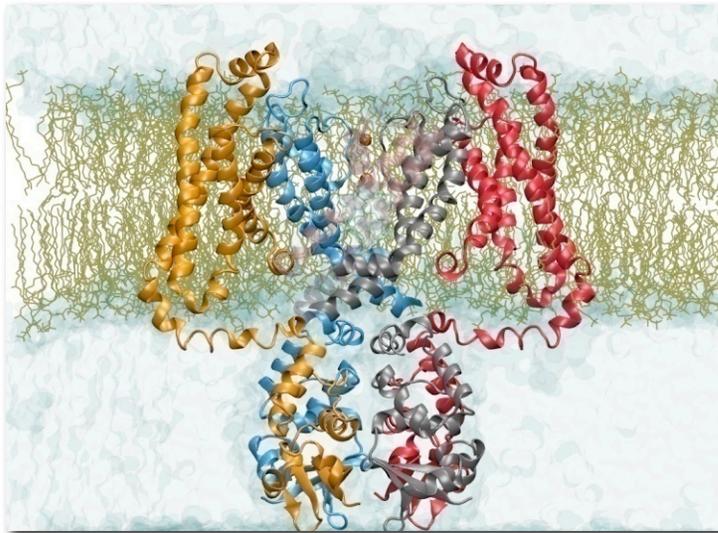
- Port of framework, Falkon, to manage run
- Falkon requires non-standard BG/P kernel (ZeptoOS)
- Huge demand on I/O system as each core is controlling multiple files
- **118,000 cores were used running nearly one million tasks**





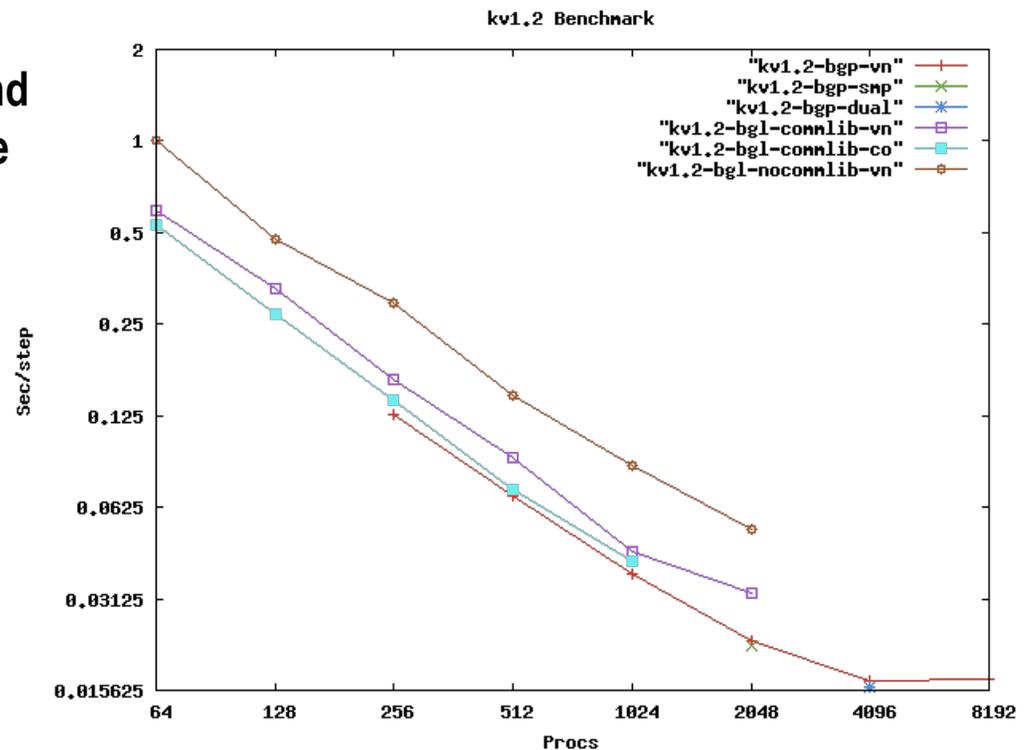
Science

- Understand how proteins work so we can alter them to change their function: micromachines
- Validated the atomic models of Kv1.2 and first to calculate the gating charge in the two functional states



Methods and Challenges

- NAMD with periodicity and particle-mesh Ewald method



kv1.2 Benchmark (352K atoms)

15-20% gain over BG/L customized ("commlib") version.



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2010 Scientific Accomplishments

What are **YOUR** Accomplishments?